



chain nodes :  
 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 31 32 35 37 38 39 40  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 10 11  
 chain bonds :  
 1-8 2-12 4-28 5-13 6-14 8-40 9-31 9-32 10-15 10-27 11-16 11-17 17-18 18-19 19-20  
 19-21 19-22 21-39 22-23 23-24 23-37 23-38 24-25 24-26 25-35  
 ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11  
 exact/norm bonds :  
 1-2 1-6 1-8 2-3 2-12 3-4 4-5 4-28 5-6 5-13 6-14 7-8 7-11 8-9 8-40 9-10 9-31  
 9-32 10-11 10-15 10-27 11-16 11-17 17-18 18-19 19-20 19-21 19-22 21-39 22-23 23-24  
 23-37 23-38 24-25 24-26 25-35

G1:O,CH2

G2:H,O,X,CH3

G3:Cb,Ak

G4:C,H

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS  
 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 31:CLASS  
 32:CLASS 35:CLASS 37:CLASS 38:CLASS 39:Atom 40:CLASS